



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 23, 2026 – 12:10 PM EDT

PDB ID : 9D95 / pdb_00009d95
Title : TCR - peptide - HLA complex
Authors : Zhu, S.; Petersen, J.; Rossjohn, J.
Deposited on : 2024-08-21
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

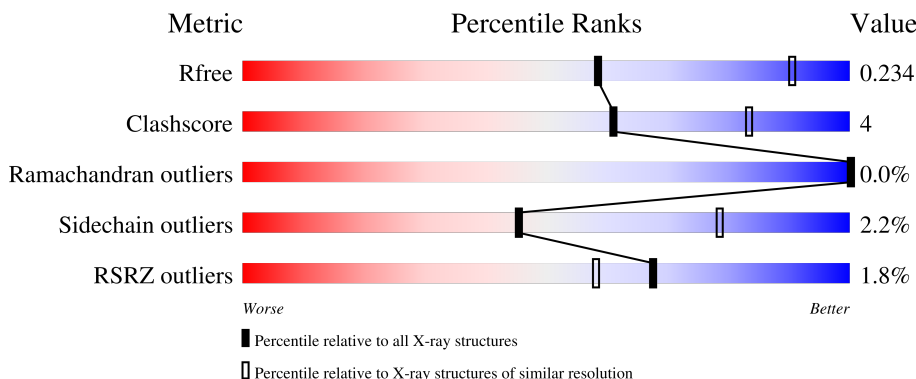
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

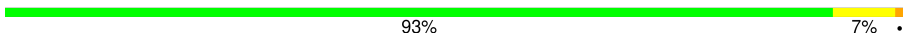
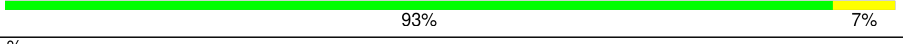
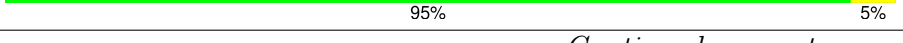
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



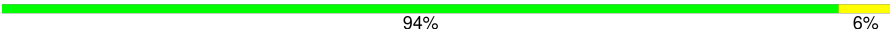
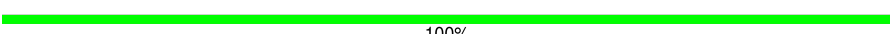
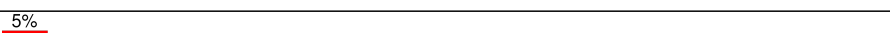
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	 93% 7%
1	F	276	 91% 9%
1	K	276	 93% 7%
1	P	276	 80% 8% 12%
2	B	100	 95% 5%

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	10	
3	H	10	
3	M	10	
3	R	10	
4	D	214	
4	I	214	
4	N	214	
4	S	214	
5	E	256	
5	J	256	
5	O	256	
5	T	256	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25533 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2256	1407	411	430	8			
1	F	276	Total	C	N	O	S	0	0	0
			2204	1377	398	422	7			
1	K	276	Total	C	N	O	S	0	1	0
			2211	1383	400	420	8			
1	P	242	Total	C	N	O	S	0	1	0
			1936	1215	349	365	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			825	527	143	151	4			
2	G	100	Total	C	N	O	S	0	0	0
			811	518	136	153	4			
2	L	100	Total	C	N	O	S	0	0	0
			809	515	137	153	4			
2	Q	100	Total	C	N	O	S	0	0	0
			794	508	137	145	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Epstein-Barr nuclear antigen 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			83	53	12	18			
3	H	10	Total	C	N	O	0	0	0
			83	53	12	18			
3	M	10	Total	C	N	O	0	0	0
			83	53	12	18			
3	R	10	Total	C	N	O	0	0	0
			83	53	12	18			

- Molecule 4 is a protein called T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	193	Total	C	N	O	S	0	0	0
			1442	913	237	284	8			
4	I	198	Total	C	N	O	S	0	0	0
			1473	935	239	291	8			
4	N	195	Total	C	N	O	S	0	0	0
			1476	934	241	292	9			
4	S	190	Total	C	N	O	S	0	0	0
			1434	914	234	280	6			

- Molecule 5 is a protein called T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1803	1138	311	345	9			
5	J	245	Total	C	N	O	S	0	0	0
			1822	1161	314	338	9			
5	O	244	Total	C	N	O	S	0	1	0
			1867	1182	326	350	9			
5	T	234	Total	C	N	O	S	0	0	0
			1711	1089	292	321	9			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



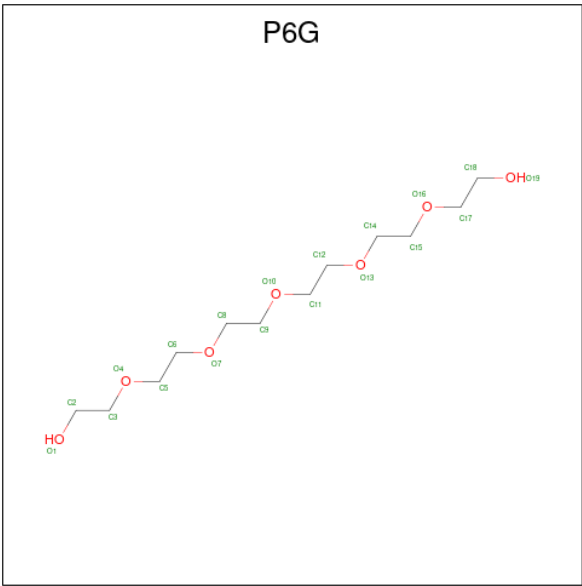
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	N	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		
7	S	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			19	12	7		
8	F	1	Total	C	O	0	0
			19	12	7		
8	K	1	Total	C	O	0	0
			19	12	7		
8	P	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	E	2	Total	O	0	0
			2	2		
9	F	2	Total	O	0	0
			2	2		
9	G	3	Total	O	0	0
			3	3		
9	H	1	Total	O	0	0
			1	1		
9	I	3	Total	O	0	0
			3	3		
9	J	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	6	Total 6	O 6	0	0
9	N	3	Total 3	O 3	0	0
9	O	2	Total 2	O 2	0	0
9	S	2	Total 2	O 2	0	0
9	T	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: MHC class I antigen

Chain A: 

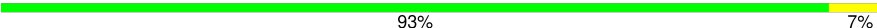


- Molecule 1: MHC class I antigen

Chain F: 



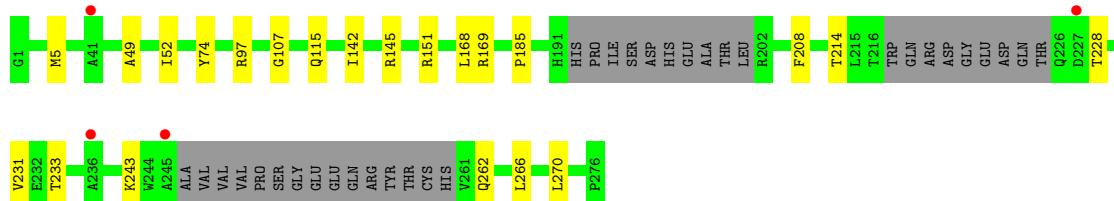
- Molecule 1: MHC class I antigen

Chain K: 

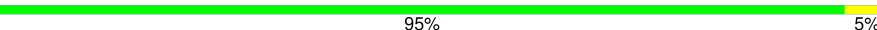


- Molecule 1: MHC class I antigen

Chain P: 



- Molecule 2: Beta-2-microglobulin

Chain B: 



- Molecule 2: Beta-2-microglobulin

Chain G: 94% 6%



- Molecule 2: Beta-2-microglobulin

Chain L: 89% 11%



- Molecule 2: Beta-2-microglobulin

Chain Q: 96%



- Molecule 3: Epstein-Barr nuclear antigen 2

Chain C: 90% 10%



- Molecule 3: Epstein-Barr nuclear antigen 2

Chain H: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Epstein-Barr nuclear antigen 2

Chain M: 90% 10%

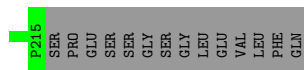
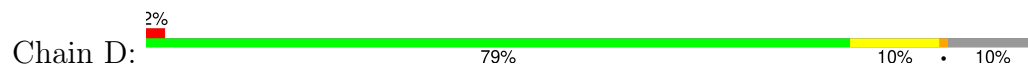


- Molecule 3: Epstein-Barr nuclear antigen 2

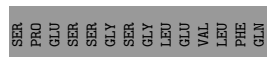
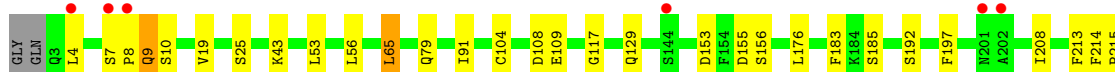
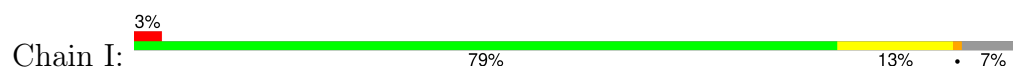
Chain R: 90% 10%



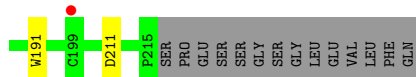
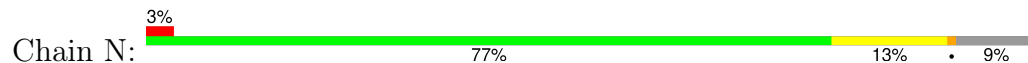
- Molecule 4: T cell receptor alpha chain



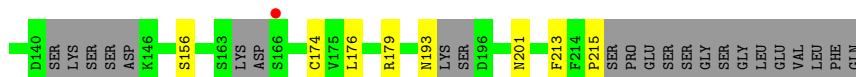
- Molecule 4: T cell receptor alpha chain



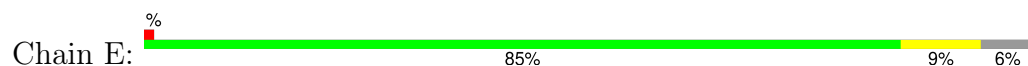
- Molecule 4: T cell receptor alpha chain

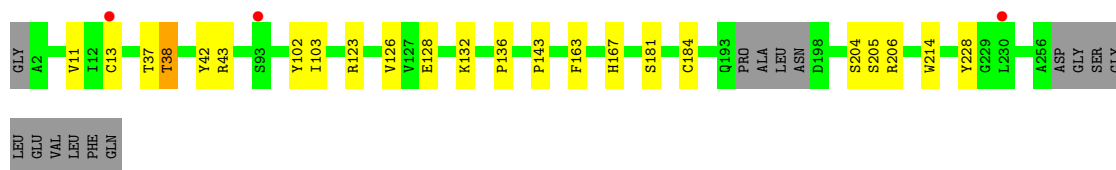


- Molecule 4: T cell receptor alpha chain

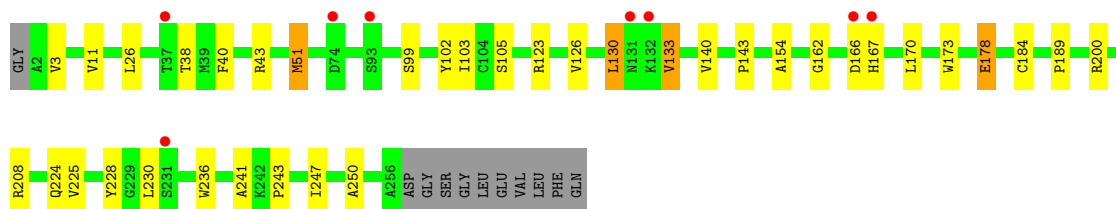
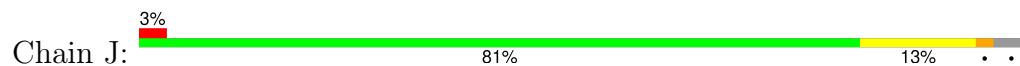


- Molecule 5: T cell receptor beta chain

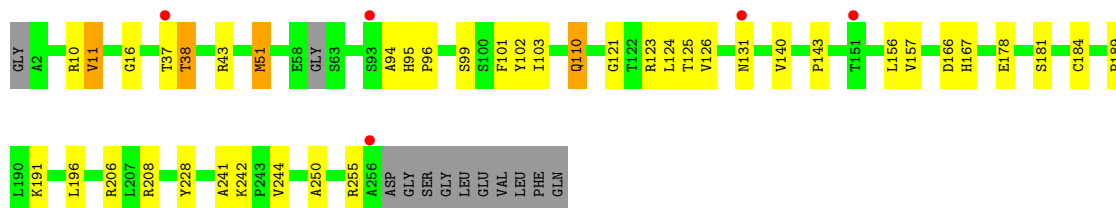
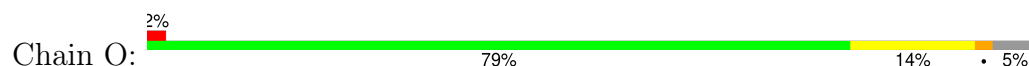




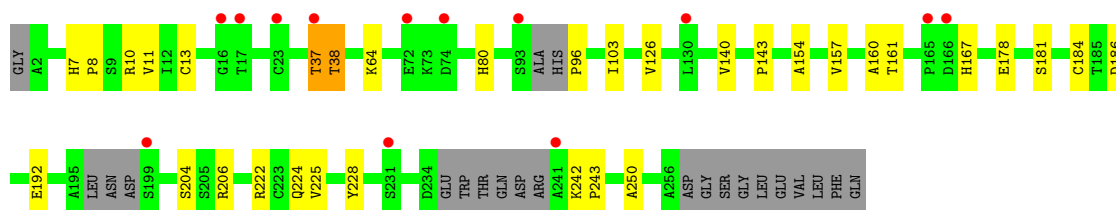
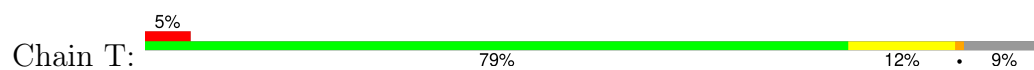
- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



- Molecule 5: T cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.79Å 124.06Å 332.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.97-2.80) 91.5 (19.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.235 0.202 , 0.234	Depositor DCC
R_{free} test set	6376 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25533	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/2322	0.24	0/3160
1	F	0.07	0/2266	0.23	0/3092
1	K	0.08	0/2276	0.24	0/3104
1	P	0.08	0/1990	0.23	0/2707
2	B	0.07	0/851	0.25	0/1152
2	G	0.07	0/834	0.26	0/1132
2	L	0.08	0/832	0.27	0/1131
2	Q	0.07	0/817	0.25	0/1112
3	C	0.12	0/84	0.25	0/113
3	H	0.07	0/84	0.25	0/113
3	M	0.07	0/84	0.20	0/113
3	R	0.08	0/84	0.27	0/113
4	D	0.09	0/1472	0.33	0/2003
4	I	0.10	0/1506	0.31	0/2055
4	N	0.10	0/1508	0.31	0/2050
4	S	0.10	0/1464	0.31	0/1989
5	E	0.09	0/1850	0.27	0/2532
5	J	0.10	0/1871	0.29	0/2562
5	O	0.08	0/1919	0.28	0/2621
5	T	0.09	0/1755	0.28	0/2400
All	All	0.08	0/25869	0.27	0/35254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2256	0	2119	12	0
1	F	2204	0	2031	14	0
1	K	2211	0	2053	12	0
1	P	1936	0	1798	11	0
2	B	825	0	789	3	0
2	G	811	0	758	6	0
2	L	809	0	747	9	0
2	Q	794	0	733	2	0
3	C	83	0	80	1	0
3	H	83	0	80	0	0
3	M	83	0	80	0	0
3	R	83	0	80	0	0
4	D	1442	0	1322	16	0
4	I	1473	0	1338	16	0
4	N	1476	0	1365	17	0
4	S	1434	0	1329	26	0
5	E	1803	0	1625	16	0
5	J	1822	0	1669	18	0
5	O	1867	0	1733	26	0
5	T	1711	0	1535	20	0
6	A	5	0	0	0	0
6	F	5	0	0	0	0
6	K	10	0	0	0	0
6	P	5	0	0	0	0
7	D	56	0	52	0	0
7	I	28	0	26	0	0
7	N	70	0	65	1	0
7	S	42	0	39	1	0
8	D	19	0	26	1	0
8	F	19	0	26	2	0
8	K	19	0	26	2	0
8	P	19	0	26	1	0
9	A	3	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	0	0
9	G	3	0	0	0	0
9	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	3	0	0	0	0
9	J	2	0	0	0	0
9	K	6	0	0	0	0
9	N	3	0	0	0	0
9	O	2	0	0	0	0
9	S	2	0	0	0	0
9	T	1	0	0	0	0
All	All	25533	0	23550	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 204 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:58:LYS:HE3	4:S:64:GLU:HG3	1.52	0.88
5:O:206[B]:ARG:HH11	5:O:206[B]:ARG:HB2	1.46	0.80
4:D:47:GLY:HA3	5:E:123:ARG:HH21	1.47	0.78
4:S:111:THR:HG23	4:S:113:LYS:H	1.49	0.75
4:I:176:LEU:HB3	5:J:184:CYS:HB2	1.72	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/276 (100%)	267 (97%)	8 (3%)	0	100	100
1	F	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	K	275/276 (100%)	268 (98%)	7 (2%)	0	100	100
1	P	235/276 (85%)	229 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	99/100 (99%)	99 (100%)	0	0	100	100
2	G	98/100 (98%)	98 (100%)	0	0	100	100
2	L	98/100 (98%)	98 (100%)	0	0	100	100
2	Q	98/100 (98%)	98 (100%)	0	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
3	M	8/10 (80%)	8 (100%)	0	0	100	100
3	R	8/10 (80%)	8 (100%)	0	0	100	100
4	D	187/214 (87%)	184 (98%)	3 (2%)	0	100	100
4	I	196/214 (92%)	191 (97%)	5 (3%)	0	100	100
4	N	191/214 (89%)	188 (98%)	3 (2%)	0	100	100
4	S	182/214 (85%)	179 (98%)	3 (2%)	0	100	100
5	E	237/256 (93%)	232 (98%)	5 (2%)	0	100	100
5	J	243/256 (95%)	235 (97%)	8 (3%)	0	100	100
5	O	241/256 (94%)	234 (97%)	6 (2%)	1 (0%)	30	60
5	T	226/256 (88%)	222 (98%)	4 (2%)	0	100	100
All	All	3187/3424 (93%)	3121 (98%)	65 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	O	241	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/237 (100%)	233 (99%)	3 (1%)	61	86
1	F	224/237 (94%)	222 (99%)	2 (1%)	70	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	226/237 (95%)	224 (99%)	2 (1%)	70	89
1	P	195/237 (82%)	193 (99%)	2 (1%)	68	88
2	B	91/95 (96%)	91 (100%)	0	100	100
2	G	89/95 (94%)	89 (100%)	0	100	100
2	L	88/95 (93%)	88 (100%)	0	100	100
2	Q	84/95 (88%)	83 (99%)	1 (1%)	63	87
3	C	10/10 (100%)	10 (100%)	0	100	100
3	H	10/10 (100%)	10 (100%)	0	100	100
3	M	10/10 (100%)	9 (90%)	1 (10%)	7	24
3	R	10/10 (100%)	9 (90%)	1 (10%)	7	24
4	D	152/188 (81%)	149 (98%)	3 (2%)	48	80
4	I	153/188 (81%)	149 (97%)	4 (3%)	40	75
4	N	159/188 (85%)	151 (95%)	8 (5%)	22	54
4	S	152/188 (81%)	145 (95%)	7 (5%)	24	58
5	E	183/223 (82%)	181 (99%)	2 (1%)	65	87
5	J	182/223 (82%)	174 (96%)	8 (4%)	25	59
5	O	194/223 (87%)	185 (95%)	9 (5%)	24	58
5	T	168/223 (75%)	163 (97%)	5 (3%)	36	72
All	All	2616/3012 (87%)	2558 (98%)	58 (2%)	45	78

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	28	ILE
5	T	38	THR
5	O	51	MET
5	T	37	THR
4	S	104	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	O	220	HIS
5	T	216	ASN
4	I	9	GLN

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Mol	Chain	Res	Type
5	J	79	ASN
5	J	216	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	N	301	4	14,14,15	1.15	1 (7%)	17,19,21	1.24	2 (11%)
8	P6G	F	301	-	18,18,18	0.11	0	17,17,17	0.08	0
7	NAG	I	301	4	14,14,15	1.13	1 (7%)	17,19,21	1.30	2 (11%)
8	P6G	P	301	-	18,18,18	0.11	0	17,17,17	0.08	0
7	NAG	D	303	4	14,14,15	0.26	0	17,19,21	0.40	0
7	NAG	S	301	4	14,14,15	0.58	0	17,19,21	0.56	0
6	SO4	F	302	-	4,4,4	0.24	0	6,6,6	0.08	0
7	NAG	N	303	4	14,14,15	0.21	0	17,19,21	0.68	0
8	P6G	D	304	-	18,18,18	0.11	0	17,17,17	0.10	0
7	NAG	S	303	4	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	N	302	4	14,14,15	0.21	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	K	302	-	4,4,4	0.24	0	6,6,6	0.10	0
7	NAG	D	302	4	14,14,15	0.33	0	17,19,21	0.51	0
7	NAG	S	302	4	14,14,15	0.46	0	17,19,21	1.38	2 (11%)
6	SO4	K	303	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.07	0
8	P6G	K	301	-	18,18,18	0.11	0	17,17,17	0.09	0
7	NAG	N	304	4	14,14,15	0.19	0	17,19,21	0.68	1 (5%)
7	NAG	N	305	4	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
7	NAG	D	301	4	14,14,15	0.59	1 (7%)	17,19,21	0.51	0
7	NAG	I	302	4	14,14,15	0.28	0	17,19,21	0.43	0
7	NAG	D	305	4	14,14,15	0.34	0	17,19,21	0.51	0
6	SO4	P	302	-	4,4,4	0.24	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	N	304	4	-	3/6/23/26	0/1/1/1
7	NAG	D	302	4	-	0/6/23/26	0/1/1/1
7	NAG	N	301	4	-	0/6/23/26	0/1/1/1
7	NAG	N	305	4	-	2/6/23/26	0/1/1/1
7	NAG	S	302	4	-	4/6/23/26	0/1/1/1
7	NAG	S	303	4	-	2/6/23/26	0/1/1/1
8	P6G	F	301	-	-	6/16/16/16	-
7	NAG	I	301	4	-	2/6/23/26	0/1/1/1
7	NAG	D	301	4	-	0/6/23/26	0/1/1/1
7	NAG	N	302	4	-	0/6/23/26	0/1/1/1
8	P6G	P	301	-	-	7/16/16/16	-
7	NAG	I	302	4	-	2/6/23/26	0/1/1/1
8	P6G	K	301	-	-	7/16/16/16	-
7	NAG	D	303	4	-	2/6/23/26	0/1/1/1
7	NAG	S	301	4	-	2/6/23/26	0/1/1/1
7	NAG	D	305	4	-	2/6/23/26	0/1/1/1
7	NAG	N	303	4	-	2/6/23/26	0/1/1/1
8	P6G	D	304	-	-	8/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	301	NAG	O5-C1	-3.68	1.37	1.43
7	N	301	NAG	O5-C1	-3.53	1.37	1.43
7	N	305	NAG	O5-C1	-2.53	1.39	1.43
7	D	301	NAG	O5-C1	-2.02	1.40	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	302	NAG	C2-N2-C7	4.52	128.96	122.90
7	N	301	NAG	C4-C3-C2	4.09	117.01	111.02
7	I	301	NAG	C4-C3-C2	3.53	116.19	111.02
7	I	301	NAG	C3-C4-C5	3.04	115.73	110.23
7	N	301	NAG	C3-C4-C5	2.75	115.21	110.23

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	301	NAG	O5-C5-C6-O6
7	D	303	NAG	O5-C5-C6-O6
7	D	303	NAG	C4-C5-C6-O6
8	K	301	P6G	O7-C8-C9-O10
8	D	304	P6G	O4-C5-C6-O7

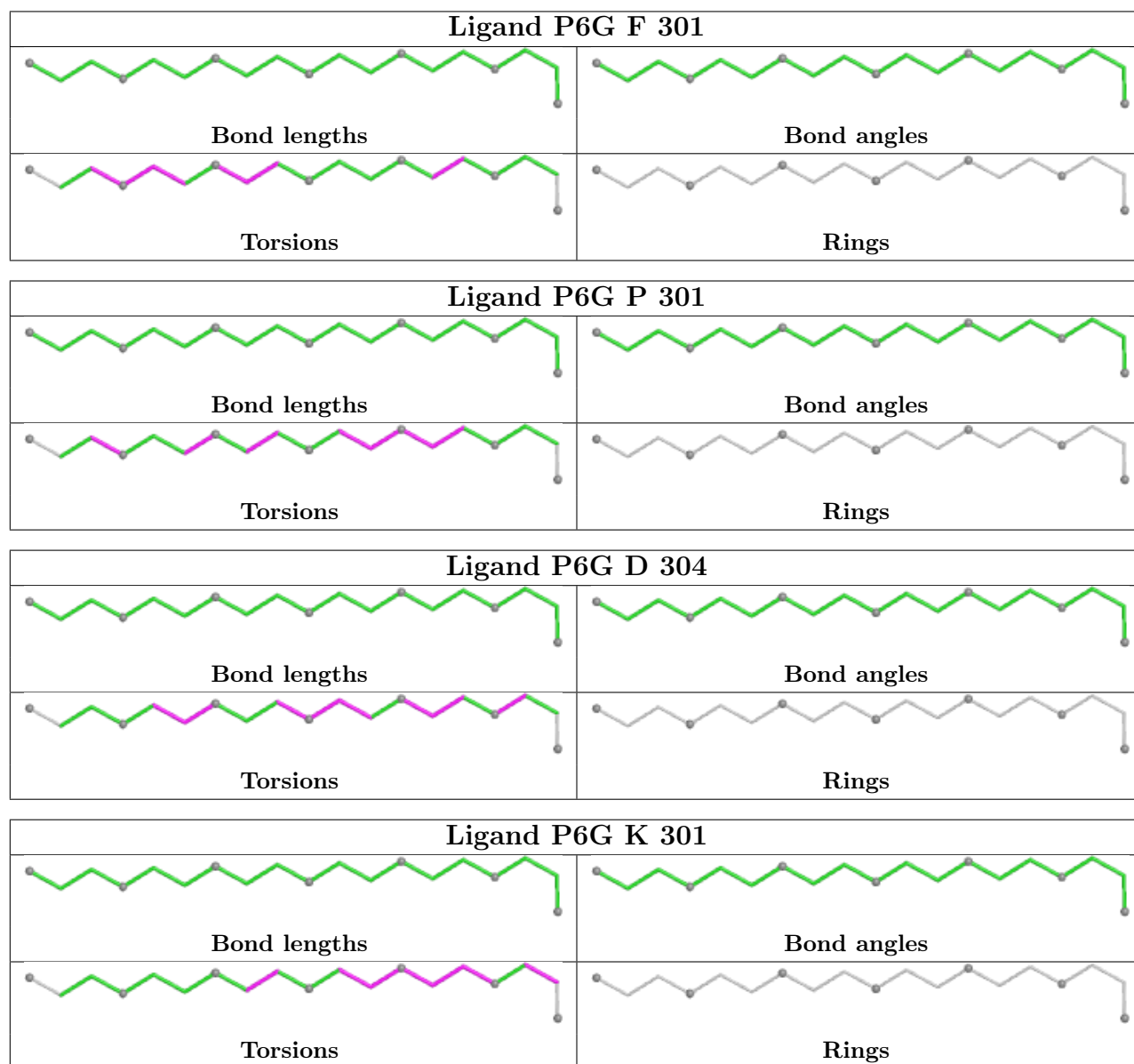
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	301	P6G	2	0
8	P	301	P6G	1	0
8	D	304	P6G	1	0
7	S	302	NAG	1	0
8	K	301	P6G	2	0
7	N	304	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	-0.20	1 (0%) 88 84	31, 56, 102, 127	1 (0%)
1	F	276/276 (100%)	-0.27	1 (0%) 88 84	31, 51, 92, 110	0
1	K	276/276 (100%)	-0.27	1 (0%) 88 84	29, 50, 86, 104	1 (0%)
1	P	242/276 (87%)	0.04	4 (1%) 69 60	33, 68, 114, 142	1 (0%)
2	B	100/100 (100%)	-0.17	0 100 100	34, 60, 91, 111	1 (1%)
2	G	100/100 (100%)	-0.26	0 100 100	38, 51, 81, 99	0
2	L	100/100 (100%)	-0.40	1 (1%) 79 72	33, 48, 77, 94	0
2	Q	100/100 (100%)	0.14	0 100 100	49, 80, 113, 123	0
3	C	10/10 (100%)	-0.26	0 100 100	42, 47, 56, 60	0
3	H	10/10 (100%)	-0.09	0 100 100	38, 42, 47, 62	0
3	M	10/10 (100%)	-0.11	0 100 100	37, 42, 45, 64	0
3	R	10/10 (100%)	-0.06	0 100 100	45, 55, 58, 70	0
4	D	193/214 (90%)	0.13	4 (2%) 63 54	38, 74, 114, 138	0
4	I	198/214 (92%)	0.18	6 (3%) 52 42	36, 65, 111, 161	0
4	N	195/214 (91%)	0.18	7 (3%) 46 37	37, 64, 98, 130	0
4	S	190/214 (88%)	0.20	4 (2%) 63 54	38, 65, 96, 121	0
5	E	241/256 (94%)	0.31	3 (1%) 76 68	43, 84, 114, 129	0
5	J	245/256 (95%)	0.27	8 (3%) 49 39	35, 74, 106, 140	0
5	O	244/256 (95%)	0.22	5 (2%) 65 56	37, 71, 97, 122	1 (0%)
5	T	234/256 (91%)	0.47	13 (5%) 30 23	40, 82, 119, 137	0
All	All	3250/3424 (94%)	0.05	58 (1%) 67 58	29, 66, 108, 161	5 (0%)

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	7	SER	5.3
4	N	166	SER	4.6
4	D	141	SER	4.4
4	I	7	SER	4.1
4	N	140	ASP	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	D	305	14/15	0.33	0.15	108,125,133,136	0
7	NAG	N	304	14/15	0.51	0.19	98,105,114,114	0
7	NAG	N	303	14/15	0.54	0.19	77,95,111,111	0
7	NAG	N	302	14/15	0.54	0.15	90,100,110,112	0
7	NAG	I	302	14/15	0.58	0.15	79,99,121,142	0
7	NAG	D	303	14/15	0.60	0.15	83,92,99,105	0
7	NAG	D	302	14/15	0.62	0.13	91,108,111,114	0
7	NAG	S	301	14/15	0.62	0.19	77,93,100,103	0
7	NAG	I	301	14/15	0.70	0.17	79,94,106,108	0
7	NAG	N	305	14/15	0.75	0.14	82,94,98,100	0
7	NAG	S	303	14/15	0.75	0.12	75,96,105,115	0
7	NAG	S	302	14/15	0.76	0.10	100,111,115,116	0
7	NAG	N	301	14/15	0.77	0.12	94,101,105,110	0
7	NAG	D	301	14/15	0.85	0.10	67,79,90,99	0
8	P6G	D	304	19/19	0.86	0.10	43,50,73,80	0
6	SO4	P	302	5/5	0.88	0.12	83,93,104,112	0
6	SO4	K	303	5/5	0.89	0.08	72,75,77,88	0
8	P6G	P	301	19/19	0.89	0.11	41,54,65,67	0
8	P6G	F	301	19/19	0.90	0.10	41,49,75,81	0

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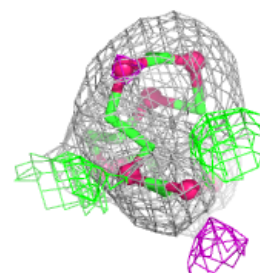
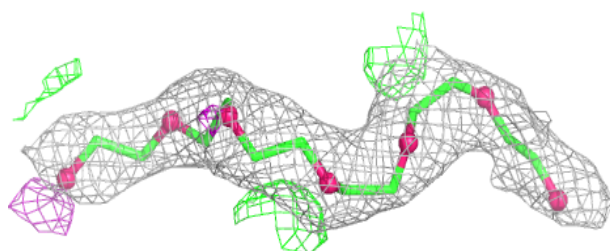
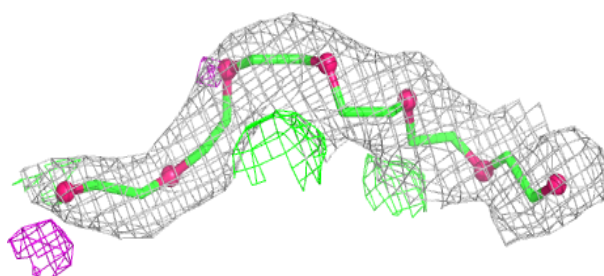
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	K	302	5/5	0.90	0.16	66,79,83,95	0
8	P6G	K	301	19/19	0.92	0.08	36,49,68,70	0
6	SO4	A	301	5/5	0.92	0.15	61,66,85,95	0
6	SO4	F	302	5/5	0.95	0.10	72,79,80,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

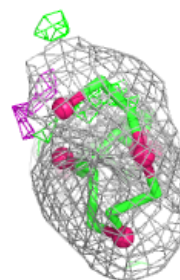
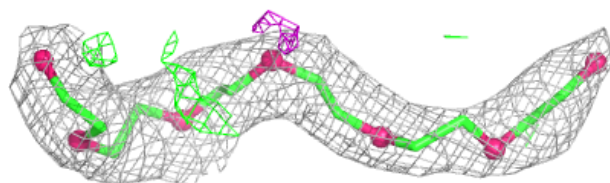
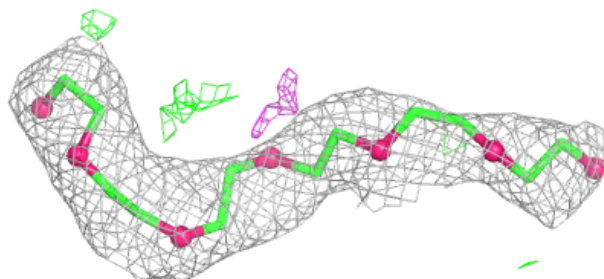
Electron density around P6G D 304:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

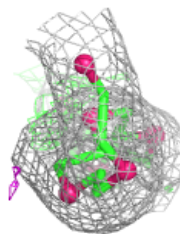
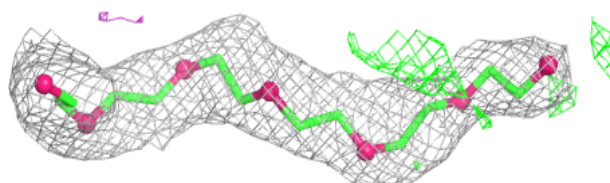
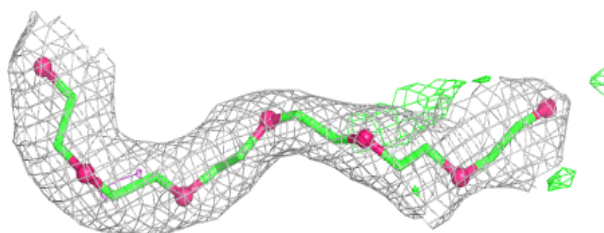


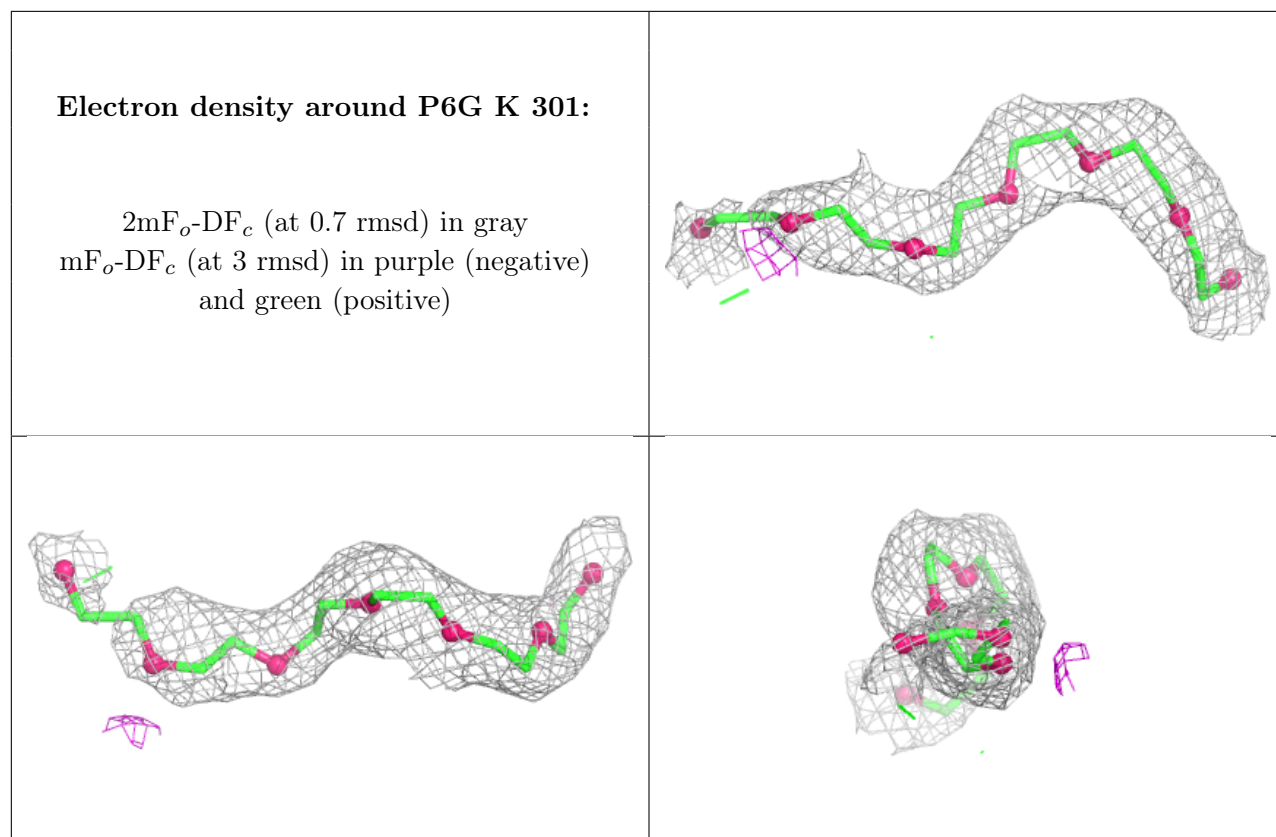
Electron density around P6G P 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around P6G F 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.